Bicyclic graphs with maximal revised Szeged index

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Abstract

The revised Szeged index $Sz^*(G)$ is defined as $Sz^*(G) = \sum_{e=uv\in E}(n_u(e)+n_0(e)/2)(n_v(e)+n_0(e)/2)$, where $n_u(e)$ and $n_v(e)$ are, respectively, the number of vertices of G lying closer to vertex u than to vertex v and the number of vertices of G lying closer to vertex v than to vertex u, and $n_0(e)$ is the number of vertices equidistant to u and v. Hansen used the AutoGraphiX and made the following conjecture about the revised Szeged index for a connected bicyclic graph G of order $n \geq 6$:

$$Sz^*(G) \leq \begin{cases} (n^3+n^2-n-1)/4, & \text{if } n \text{ is odd,} \\ (n^3+n^2-n)/4, & \text{if } n \text{ is even.} \end{cases}$$

with equality if and only if G is the graph obtained from the cycle C_{n-1} by duplicating a single vertex. This paper is to give a confirmative proof to this conjecture.

Keywords: Wiener index, Szeged index, Revised Szeged index, bicyclic graph.

AMS subject classification 2010: 05C12, 05C35, 05C90, 92E10.

1 Introduction

All graphs considered in this paper are finite, undirected and simple. We refer the readers to [2] for terminology and notations. Let G be a connected graph with vertex set V and edge set E. For $u, v \in V, d(u,v)$ denotes the distance between u and v. The *Wiener index* of G is defined as

$$W(G) = \sum_{\{u,v\}\subseteq V} d(u,v).$$

This topological index has been extensively studied in the mathematical literature; see, e.g., [4, 6]. Let $e = uv$ be an edge of G, and define three sets as follows:

$$N_u(e) = \{w \in V : d(u,w) < d(v,w)\},$$

$$N_v(e) = \{w \in V : d(v,w) < d(u,w)\},$$
$$N_0(e) = \{w \in V : d(u,w) = d(v,w)\}.$$

Thus, $\{N_u(e), N_v(e), N_0(e)\}$ is a partition of the vertices of G respect to e. The number of vertices of $N_u(e)$, $N_v(e)$ and $N_0(e)$ are denoted by $n_u(e)$, $n_v(e)$ and $n_0(e)$, respectively. A long time known property of the Wiener index is the formula [5, 12]:

$$W(G) = \sum_{e=uv\in E} n_u(e)n_v(e),$$

which is applicable for trees. Using the above formula, Gutman [3] introduced a graph invariant named the *Szeged index* as an extention of the Wiener index and defined it by

$$Sz(G) = \sum_{e=uv\in E} n_u(e)n_v(e).$$

Randić [10] observed that the Szeged index does not take into account the contributions of the vertices at equal distaances from the endpoints of an edge, and so he conceived a modified version of the Szeged index which is named the *revised Szeged index*. The revised Szeged index of a connected graph G is defined as

$$Sz^*(G) = \sum_{e=uv\in E} \left(n_u(e) + \frac{n_0(e)}{2}\right)\left(n_v(e) + \frac{n_0(e)}{2}\right).$$

Some properties and applications of this topological index have been reported in [8, 9]. In [1], Aouchiche and Hansen showed that for a connected graph G of order n and size m, an upper bound of the revised Szeged index of G is $\frac{n^2m}{4}$. In [13], Xing and Zhou determined the unicyclic graphs of order n with the smallest and the largest revised Szeged indices for $n \geq 5$, and they also determined the unicyclic graphs of order n with a unique cycle of length r $(3 \leq r \leq n)$, with the smallest and the largest revised Szeged indices.

In [7], Hansen used the AutoGraphiX and made the following conjecture:

Conjecture 1.1 *Let G be a connected bicyclic graph G of order $n \geq 6$. Then*

$$Sz^*(G) \leq \begin{cases} (n^3+n^2-n-1)/4, & \text{if } n \text{ is odd,} \\ (n^3+n^2-n)/4, & \text{if } n \text{ is even.} \end{cases}$$

with equality if and only if G is the graph obtained from the cycle C_{n-1} by duplicating a single vertex (see Figure 1).

It is easy to see that for bicyclic graphs, the upper bound in Conjecture 1.1 is better than $\frac{n^2m}{4}$ for general graphs.

This paper is to give a confirmative proof to this conjecture.

2 Main results

For convenience, let B_n be the graph obtained from the cycle C_{n-1} by duplicating a single vertex (see Figure 1). It is easy to check that

$$Sz^*(B_n) = \begin{cases} (n^3+n^2-n-1)/4, & \text{if } n \text{ is odd,} \\ (n^3+n^2-n)/4, & \text{if } n \text{ is even.} \end{cases}$$

i.e., B_n satisfies the equality of Conjecture 1.1.

So, we are left to show that for any connected bicyclic graph G_n of order n, other than B_n, $Sz^*(G_n) < Sz^*(B_n)$. Using the fact that $n_u(e)+n_v(e)+n_0(e)=n$, we have

$$\begin{aligned} Sz^*(G) &= \sum_{e=uv\in E}\left(n_u(e)+\frac{n_0(e)}{2}\right)\left(n_v(e)+\frac{n_0(e)}{2}\right) \\ &= \sum_{e=uv\in E}\left(\frac{n+n_u(e)-n_v(e)}{2}\right)\left(\frac{n-n_u(e)+n_v(e)}{2}\right) \\ &= \sum_{e=uv\in E}\frac{n^2-(n_u(e)-n_v(e))^2}{4} \\ &= \frac{mn^2}{4}-\frac{1}{4}\sum_{e=uv\in E}(n_u(e)-n_v(e))^2. \end{aligned}$$

Moreover, from $m=n+1$ we have

$$Sz^*(G) = \frac{n^3+n^2}{4}-\frac{1}{4}\sum_{e=uv\in E}(n_u(e)-n_v(e))^2 \tag{1}$$

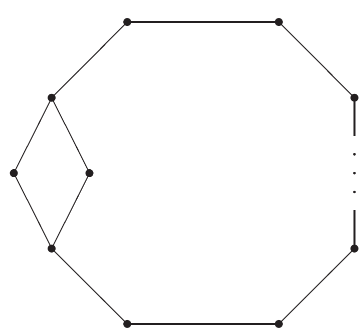

Figure 1: B_n

We distinguish three cases to show the conjecture. First, we consider connected bicyclic graphs with at least one pendant edge. Then, we consider connected bicyclic graphs without pendant edges but with a cut vertex. Finally, we consider 2-connected bicyclic graphs. In the following lemmas, we deal with these cases separately.

Lemma 2.1 *Let G_n be a connected bicyclic graph of order $n \geq 6$ with at least one pendant edge, i.e., $\delta(G_n) = 1$. Then*

$$Sz^*(G_n) < Sz^*(B_n)$$

Proof. Let $e' = xy$ be a pendant edge and $d(y) = 1$. Then, for $n \geq 6$, we have

$$\begin{aligned}
\sum_{e=uv\in E} (n_u(e) - n_v(e))^2 &\geq (n_x(e') - n_y(e'))^2 \\
&= (n-1-1)^2 \\
&> n+1.
\end{aligned}$$

Combining with equality (1), the result follows. ∎

Lemma 2.2 *Let G_n be a connected bicyclic graph of order $n \geq 6$ without pendant edges but with a cut vertex, i.e., $\delta(G_n) \geq 2$ and $\kappa(G_n) = 1$. Then, we have*

$$Sz^*(G_n) < Sz^*(B_n)$$

Proof. Since $\delta(G_n) \geq 2$ and $\kappa(G_n) = 1$, G_n consists of two disjoint cycles linked by a path or two cycles with a common vertex. Assume that C_1 and C_2 are the two cycles of G_n, P_t is the path joining C_1 and C_2, where $t \geq 0$ is the length of the path. Thus $|C_1| + |C_2| + t - 1 = n$, and $|C_1| \geq 3$ and $|C_2| \geq 3$. Let $u \in C_1$, $v \in C_2$ be the endpoints of P_t. Now we consider the four edges on the two cycles which are incident with u and v. Without loss of generality, we consider one of the 4 edges $e_1 = uw$. Then we have

$$n_u(e_1) - n_w(e_1) = n - |C_1| + \left\lfloor \frac{C_1}{2} \right\rfloor - \left\lfloor \frac{C_1}{2} \right\rfloor = n - |C_1|$$

For the other three edges, one can get equalities similar to the above. So we have, for $n \geq 6$,

$$\begin{aligned}
\sum_{e=uv\in E} (n_u(e) - n_v(e))^2 &\geq 2(n - |C_1|)^2 + 2(n - |C_2|)^2 \\
&= 2\left(2nt - 2n + |C_1|^2 + |C_2|^2\right) \\
&\geq 2\left(2nt - 2n + 2 \times \left(\frac{n+1-t}{2}\right)^2\right) \\
&= (n-1+t)^2 \\
&> n+1,
\end{aligned}$$

Combining with equality (1), this completes the proof. ∎

For the last case, i.e., $\kappa(G_n) \geq 2$, we define a class of graphs. A graph is called a Θ-graph if it consists of three internally disjoint paths connecting two fixed vertices. Obviously, in this case G_n must be a Θ-graph.

Lemma 2.3 *Let $G = (V, E)$ be a Θ-graph, $e = uv \in E$. Then $|n_u(e) - n_v(e)| = 0$ if and only if e is placed in the middle position of an odd path of G.*

Proof. Assume that x and y are the vertices in G with degree 3, and $e = uv$ belongs to P_i $(1 \leq i \leq 3)$, the ith path connecting x and y. Then, with respect to $N_u(e)$ and $N_v(e)$, there are three cases to discuss.

Case 1. x, y are in different sets. We claim that

$$|n_u(e) - n_v(e)| = |b_i - a_i|,$$

where a_i (resp. (b_i)) is the distance between x (resp. y) and the edge e.

To see this, assume that $x \in N_u(e),\ y \in N_v(e)$. Then we have $a_i - b_i$ vertices more in $N_u(e)$ than in $N_v(e)$ on the path P_i, but on each path P_j $(j \neq i)$, we have $b_i - a_i$ vertices more in $N_u(e)$ than in $N_v(e)$. Hence $|n_u(e) - n_v(e)| = |2(b_i - a_i) + (a_i - b_i)| = |b_i - a_i|$.

Case 2. x, y are in the same set. We claim that

$$|n_u(e) - n_v(e)| = |V| - g,$$

where g is the length of the shortest cycle of G that contains e.

To see this, assume that $x, y \in N_u(e)$. Thus all vertices from the paths P_i $(j \neq i)$ are in $N_u(e)$. Therefore, $n_v(e) = \lfloor \frac{g}{2} \rfloor$, while $n_u(e) = \lfloor \frac{g}{2} \rfloor + |V| - g$. So $|n_u(e) - n_v(e)| = |V| - g$.

Case 3. one of x, y is in $N_0(e)$. We claim that

$$|n_u(e) - n_v(e)| \geq a - 1,$$

with equality if and only if G has two paths of length a, where a is the length of a shortest path of G.

To see this, assume that $x \in N_u(e)$, $y \in N_0(e)$. Then the shortest cycle C of G that contains e is odd. Let $z \in V \backslash C$ be the furthest vertex from e such that $z \in N_0(e)$. Then $|n_u(e) - n_v(e)| = d(x, z) - 1 \geq a + d(y, z) - 1 \geq a - 1$.

From the above, we know that $|n_u(e) - n_v(e)| \geq 1$ in Case 2. In Case 3, $|n_u(e) - n_v(e)| = 0$ if G has two paths of length 1, which is impossible since G is simple. So, $|n_u(e) - n_v(e)| = 0$ if and only if x, y are in different sets and $|b_i - a_i| = 0$, that is, e is placed in the middle position of an odd path of G. ∎

Now we are ready to give our main result.

Theorem 2.4 *If G_n is a connected bicyclic graph of order $n > 6$, other than B_n, then*

$$Sz^*(G_n) < Sz^*(B_n).$$

Proof. The result follows from Lemmas 2.1 and 2.2 for bicyclic graphs of connectivity 1. So, we assume that G_n is 2-connected next. Then G_n must be a Θ-graph. Let x and y be the vertices in G with degree 3, $a \leq b \leq c$ be the lengths of the corresponding 3 paths. By Lemma 2.3, we know that there are at most 3 edges such that $|n_u(e) - n_v(e)| = 0$. We distinguish the following cases to proceed the proof.

Case 1. $3 \leq a \leq b \leq c$.

Consider the six edges which are incident with x and y. Let $e_1 = xz$ be one of them. Then, $|n_u(e) - n_v(e)| \geq 2$ from Lemma 2.3. Similar thing is true for the other five edges. Hence

$$\sum_{e=uv \in E} (n_u(e) - n_v(e))^2 \geq 2^2 \times 6 + (m - 6 - 3) = m + 15 > m = n + 1.$$

Combining with equality (1), the result follows.

Case 2. $2 = a < b \leq c$.

Consider the four edges which are incident with x and y but do not belong to the shortest path. Let $e_1 = xz$ be one of them. Then, $|n_u(e) - n_v(e)| \geq 2$ from Lemma 2.3. Similarly, this is true for the other three edges. Hence,

$$\sum_{e=uv \in E} (n_u(e) - n_v(e))^2 \geq 2^2 \times 4 + (m - 4 - 2) = m + 10 > m = n + 1.$$

Combining with equality (1), the result follows.

Case 3. $1 = a < b \leq c$.

If $b \geq 3$, similar to the above Case 2, we have

$$\sum_{e=uv \in E} (n_u(e) - n_v(e))^2 \geq 2^2 \times 4 + (m - 4 - 3) = m + 9 > m = n + 1.$$

Combining with equality (1), the result follows.

If $b = 2$, we consider the two edges on the second longest path. Let $e_1 = xw$ be one of them. Obviously, $y \in N_0(e)$, in other words, $|n_u(e) - n_v(e)| = d(x, z) - 1 \geq a + d(y, z) - 1 = d(y, z)$, where z is defined as in Case 3 of Lemma 2.3. We claim that $d(x, z) \geq 3$. Otherwise, if $d(x, z) \leq 2$, then $d(y, z) \leq 1$, thus $c = d(x, z) + d(y, z) \leq 3$. It follows that $n = a + b + c - 1 \leq 5$, a contradiction. Now we have

$$\sum_{e=uv \in E} (n_u(e) - n_v(e))^2 \geq 2^2 \times 2 + (m - 2 - 2) = m + 4 > m = n + 1.$$

Combining with equality (1), the result follows. ∎

According to our proof for Conjecture 1.1, we can also get that among connected bicyclic graphs of order n, the graph $\Theta(1, 2, n-2)$ has the second-largest revised Szeged index, where $\Theta(a, b, c)$ is a Θ-graph with three paths of lengths a, b, c, respectively.

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